## 研究・成果概要

**Kinetic Monte Carlo model of dislocation motion in dilute iron-based alloy**


### Atomic model to coarse grained kMC model

- Screw dislocation described as line segments
- Each segment has a length of a certain Burgers vector
- Dislocation segment moves on (110) slip plane along [112] direction

**Algorithm of kMC simulation**

1. Construct the event list
2. Calculate the total rate of event list
3. Select the event from possible event list
4. Execute the selected event
5. Update the time with $\Delta t = 1/P$
6. Update event list

**Activation energy on dislocation motion**

- Solute effect on double kink nucleation
- Solute effect on kink migration process

**Modeling of solute-dislocation interaction**

- Solute effect: change in total interaction energy on each state
- Distribution of $\Delta U$

**Solute effect on dislocation velocity**

- Activation energy on dislocation motion with solute effect
- Solute addition reduces the temperature dependence of CRSS at high temperature

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### 構造材料（合金）の機械的特性の制御や予測

### 最終目標

様々な合金に対するハミルトニアンからの強度予測結果を用いることで実現する、機械学習を用いた合金強度設計

### 産業界への期待・要望

マルチスケールモデリングが高度化し、その有用性が近年高まってきており、材料開発に積極的に用いてほしい